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ClayFF and Recent Developments in Atomistic Computational Modeling of Geomaterials and their Fluid Interfaces

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Molecular-level knowledge of the thermodynamic, structural, and transport properties of aqueous and non-aqueous fluids confined in nanopores and at interfaces with clays and other nanostructured geomaterials is crucial for quantitative understanding and prediction of many processes in nature and in various technological applications, including mineral weathering, geological carbon sequestration, water desalination, geological disposal and storage of radioactive waste, etc. Modern methods of atomistic computational modeling are capable to significantly complement the experimentally developed nano-scale picture of such systems by providing a detailed self-consistent description of the structural, thermodynamic, spectroscopic, transport, and other properties of such materials. This, in turn, can lead to a greatly improved molecular-scale understanding of the specific effects of the mineral substrate structure and composition on the structure, dynamics and reactivity of the interfacial and nano-confined fluid phases.

However, accurate and realistic molecular scale computer simulations of geomaterials are often particularly challenging because of the great diversity of their chemical composition, the significant degree of their structural and compositional disorder. ClayFF was originally developed over 20 years ago in response to a strong need for a robust and flexible force field for classical atomistic simulations of geomaterials and their fluid interfaces, as well as their interactions with various inorganic and organic dissolved species [1]. This talk will provide a brief overview of the fundamental assumptions and limitations of the ClayFF approach to the atomistic modeling of geomaterials, focusing on the most recent improvements and advances, illustrated by select examples representing a wide range of geochemical, environmental, and energy applications [2-5].

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